Concept of Fractals in Mathematical Modeling on Management of Adsorption Processes

Ali Nagiev[1], Fazil Alekperli[2], Jabir Mamedov[3]
[1,2]Sumgait State University, Sumgait, Azerbaijan
[3]Azerbaijan High Military School named after Heydar Aliyev, Baku, Azerbaijan
[1]*nashfn@hotbox.ru*, [2]*fazlf@mail.ru*, [3]*cabir_m@mail.ru*

***Abstract*— A mathematical model for managing the adsorption process, compiled based on the concept of fractals. As a fractal structure used a branching-tree unit, called dendrites. We derive the differential equations of mass transfer and adsorption in micro-channels that make up the dendritic structure.**

Keywords*— *mathematical modeling; fractals; dendritic formation; adsorption; diffusion

I. INTRODUCTION

Recently, in the mathematical modeling of physical processes in computer graphics and in other areas of scientific investigation, attention to the concept of fractals increased. Active attempts have been made to use this concept to describe the internal structures of highly porous materials that are highly effective adsorbents. Finding a certain order in the clusters packing formed from similar small-scale clusters, investigators have come to a conclusion about the fractality of the structure of a porous medium [1].

By the definition given by B.Mandelbrot [2] - the founder of fractal geometry, a fractal is a structure consisting of parts similar to the whole. The contours of hills, clouds, sea coasts, snowflake curves, soot flakes, and the structure of the vascular systems in organisms are fractal.

In the practical application of fractal geometry in the investigation of technical systems, a fractal, which is an abstract Cantor set of segment parts [0,1], was widely used [3]. Taking a singular segment as the initial element and dividing it at every iteration into three equal parts, removing in this case the middle part, it is possible to obtain an infinite series of quotients tending to zero from the division (Fig. 1). It is obvious that at the *n*-th step, we will have 2n segments of 1/3n-length each. At *n*=1,2,3,…, we obtain a set of segments 1,2/3,4/9,8/27,… tending to infinity. The overall length of the segments for any $\delta(n) = (1/3)^n$ is determined by the relation:

$$\ell(n) = \delta^d(n)\left(\frac{\ell_0}{\delta(n)}\right)^D. \qquad (1)$$

This type of formula is observable in regards to the fact that the order of the first multiplier d can be compared to the order of the second multiplier D.

The value of d is a topological dimension of space, in which the segments of $\delta(n)$ length are determined (in this case, $d=1$; for a planar geometric figure, $d=2$; and for the space, $d=3$), and the value of d is a fractal dimension of the Cantor space.

The fractal dimension D for this set is calculated by the equation (2):

$$D = \frac{\ln\frac{N(\delta)}{N(\delta')}}{\ln\frac{\delta'}{\delta}} = \frac{\ln 2}{\ln 3} \approx 0.6309, \qquad (2)$$

where $N(\delta), N(\delta') -$ are, respectively, the number of the fractal covering by elements of the given characteristic size (scale index) δ at some iteration n, and the characteristic size $\delta' = \frac{1}{3}\delta$ at the following iteration $n+1$.

If we extend the representation about such a singular Cantor segment and add two additional spatial dimensions, then it is possible to proceed to the statements about some tube of a single volume $v_0 = 1$ with the initial radius r_0. The length of the tube will be $\ell_0 = \frac{1}{\pi r_0^2}$. Leaving the rule of the formation of tubes unchanged, we obtain a sequence of threefold decreased volumes: $v_1 = \pi r_1^2 \ell_1 = \frac{1}{3}$, $v_2 = \pi r_2^2 \ell_2 = \frac{1}{9}$.... The number of tubes in every generation will also be 2^n. The overall volume of one generation at every iteration will be decreased by $\frac{2}{3}$ times. In this case, as can be readily noted, we have a Cantor set of geometrical dimensions of the spatial objects. Let the scale index be the tube radius.

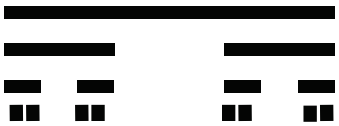

Fig. 1. Triad cantor set of the segments [0,1].

Turning to the spatial objects, we obtain the possibility of choosing the rule of the assignment of the radius definition at every iteration, $r_{n+1} = ar_n$; $0 < a < 1$; in this case leaving, for example, the description of the formation rule of a new generation of tubes with a threefold decreased volume unchanged. Then, the length of each tube in the new iteration should be determined as $\ell_{n+1} = \frac{1}{3a^2}\ell_n$. In this case, the set dimension of the fractal spatial objects relative to the value of v (volume carrier) will not obviously differ from $D = \frac{\ln 2}{\ln 3}$ previously calculated from the one-dimensional Cantor set, regardless of the value of a.

Now let us imagine that the Cantor set consists of a sequence of values $s_n = \pi r_n \ell_n$ expressing the area of these tube surfaces (tubes with walls of zero thickness). In this case, the carrier of the fractal dimension will be mentioned area.

Thus, the sequence of geometrical dimensions of the forming spatial objects, contrary to the Cantor set of one-dimensional elements, can be characterized by a series of fractal dimensions; in this case, by the volume carrier, the surface area, and the perimeter of the tube (channel). Both the radius and channel length can be used as the scale index. To be specific, further we use only the radius.

II. The Tree-Like Branching Aggregate – the Fractal Dendrite

Let us consider the problems of the supplement to the modeling of concrete porous structures. As the Cantor spatial objects, let us accept a tree-like branching aggregate – dendrite (Fig. 2a). Figure 2b shows the scheme of the development of the dendrite aggregates on the surface of the porous grain material. As the object of modeling, we will consider some dendrites with the determined parameters of the inlet r_0, v_0. In this case, we take into account that the condition $\frac{v_{n+1}}{v_n} < 1$ is satisfied, and, in addition, we keep in mind that : $a = \frac{r_{n+1}}{r_n} = \frac{\ell_{n+1}}{\ell_n}$ and $\frac{r_n}{\ell_n} = b$. Let us also give the relation $\frac{\chi_{n+1}}{\chi_n} = c$, the amount of branches on the dendrite stalk,

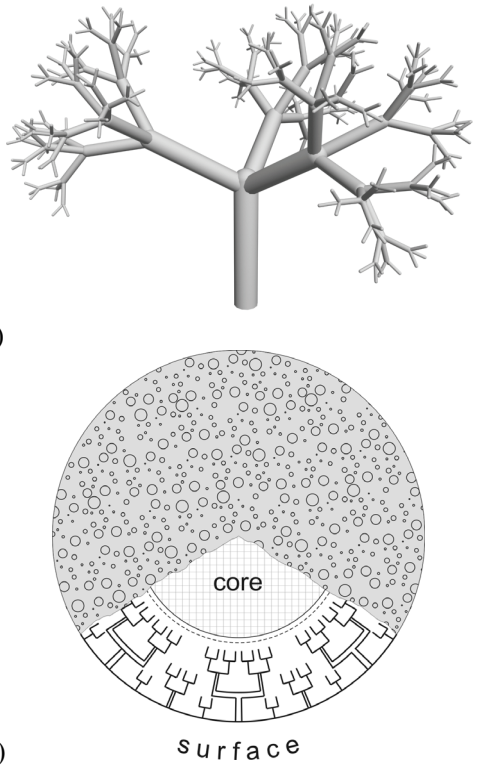

Fig. 2. The dendrite model of a porous material.
a) the dendrite formation in five generations of branches
b) the location of the pores inside of the grains

where χ_n, χ_{n+1} – are the amounts of dendrite branches in the corresponding generations with the numbers $n, n+1$. In addition, let us accept that $0 < a < 1; 0 < b < 1; c > 1$.

Let us we write the following relations:

$$\frac{V_n}{V_{n+1}} = \frac{\pi r_n^2 \ell_n}{\pi r_{n+1}^2 \ell_{n+1}} = \frac{\pi r_n^2 \ell_n}{\pi a^2 r_n^2 b \ell_n} = \frac{1}{a^2 b} = k_v^3; \quad k_v = (a^2 b)^{-\frac{1}{3}}, \qquad (3)$$

where k_V^3 – is the number of the cower of the volume of some fractal element with the generation number n by the elements in the scale of the following generation $n+1$. Due to this, the scale characterizing the elements of the given generation n will be determined in the following way:

$$\delta_v(n) = \left(\frac{1}{k_V}\right)^n = \left(a^2 b\right)^{n/3}. \qquad (4)$$

Similarly, let us determine the scales of the carries of the surface and perimeter of the dendrite branch sections in the generation n:

$$\frac{S_n}{S_{n+1}} = \frac{2\pi r_n \ell_n}{2\pi r_{n+1}\ell_{n+1}} = \frac{1}{ab} = k_S^2; \quad k_S = (ab)^{-\frac{1}{2}},$$
$$\delta_S(n) = \left(\frac{1}{k_S}\right)^n = (ab)^{n/2} \tag{5}$$

$$\frac{\Pi_n}{\Pi_{n+1}} = \frac{2\pi r_n}{2\pi r_{n+1}} = \frac{1}{a} = k_\Pi;$$
$$\delta_\Pi(n) = \left(\frac{1}{k_\Pi}\right)^n = a^n \tag{6}$$

Let us determine the fractal dimension of the volume carrier according to Eq. (2) in the following form:

$$D_V = \frac{\ln\frac{N(\delta(n+1))}{N(\delta(n))}}{\ln\frac{\delta(n)}{\delta(n+1)}} = \frac{\ln\left(k_v^3 + c\right)}{\ln k_v} = \\ = -\frac{\ln\left(\frac{1}{a^2 b} + c\right)}{\frac{2}{3}\ln a + \frac{1}{3}\ln b}, \tag{7}$$

and also by the carries of the contact surface and section perimeter by applying the corresponding expressions:

$$D_S = -\frac{\ln\left(\frac{1}{ab} + c\right)}{\frac{1}{2}\ln a + \frac{1}{2}\ln b}, \quad D_\Pi = -\frac{\ln\left(\frac{1}{a} + c\right)}{\ln a}. \tag{8}$$

Let us write the equations for the determination of the total volume, channel surface area, and total perimeters of the dendrite sections for an arbitrary given scale δ:

$$V(\delta) = \delta^3\left(\frac{V_0^{\frac{1}{3}}}{\delta}\right)^{D_V}; \quad S(\delta) = \delta^2\left(\frac{S_0^{\frac{1}{2}}}{\delta}\right)^{D_S}; \\ \Pi(\delta) = \delta\left(\frac{\Pi_0}{\delta}\right)^{D_\Pi}. \tag{9}$$

Expressing the carrier scale by length of the dendrite branch for an arbitrary generation ℓ, and also performing the differentiation with respect to ℓ, we obtain the differential functions of the distribution of the total perimeters and the total sectional areas by the scale ℓ:

$$\Pi'(\ell) = f_{\Pi\ell} b R_0 (D_\Pi - 1)\left(\frac{bR_0}{\ell}\right)^{D_\Pi - 2}; \\ S'(\ell) = \frac{dS(\ell)}{d\ell} = f_{S\ell} b^2 R_0^2 (D_S - 2)\left(\frac{bR_0}{\ell}\right)^{D_S - 3} \tag{10}$$

III. The Model of the Mass Transfer in the Fractal Medium

From a practical point of view of function (10) express the differential distribution law in the natural scale of measurement parameters porometric viewed in magnitude ℓ. They differ from the standard distribution functions is that they are defined in Cantor sets of variable (as well as parameters Π, S, V), which was originally introduced as a set of isolated points of the real axis.

Establish a connection between the physical measure of the space extension in the usual metric ε and overall length of the channels to the number of generations n, inclusive. To do this, taking as a continuous variable n, we integrate the following expression:

$$\varepsilon(n) = \ell_0 \int_0^n a^\xi d\xi = \frac{\ell_0}{\ln a}(a^n - 1), \quad a < 1, \tag{11}$$

hence it is easy to obtain:

$$\varepsilon_{\max} = \varepsilon(\infty) = -\frac{\ell_0}{\ln a}. \tag{12}$$

Let us consider the parallel diffusion mass transfer and adsorption processes in a single dendrite. We use the concept of "pseudo-channel" as a tools to obtain the corresponding differential equations involving the distribution function (10). The physical measure of the space extension defined by (11) is the longitudinal coordinate of the channel.

Write a differential equation of non-stationary diffusion processes in the volume can be based on Fick's first law. A parallel process of adsorption can be written on the basis of monomolecular Langmuir mechanism.

Below is a system of two differential equations expressing the mass transfer processes in the gas (in the pores) and solid (on the walls of channels) phases:

$$\frac{S'(\varepsilon)}{RT_0}\frac{\partial P(t,\varepsilon)}{\partial t} = D_{dif}\frac{\partial}{\partial\varepsilon}\left[S(\varepsilon)\frac{\partial}{\partial\varepsilon}P(t,\varepsilon)\right] - \\ - k_a P(t,\varepsilon)(1-n)\sigma\Pi'(\varepsilon) + k_d n\sigma\Pi'(\varepsilon) \\ \frac{\partial n(t,\varepsilon)}{\partial t} = k_a P(t,\varepsilon)\left[1 - n(t,\varepsilon)\right] - k_d n(t,\varepsilon) \tag{13}$$

where D_{dif} – the diffusion coefficient, P – the partial pressure, R – the universal gas constant, T_0 – the standard temperature, σ – the amount of the adsorption centers on the surface area unit, n – the occupied fractions of the adsorption centers, k_a, k_d – the constants rate of adsorption and desorption processes.

The initial conditions for the model (13) the following expressions:

$$t = 0, \quad P(0,\varepsilon) \equiv 0; n(0,\varepsilon) \equiv 0; \tag{14}$$

The conditions expressing stationary concentrations of the compounds in the flow of the gas phase and the zero concentrations of the compounds in the core inaccessible for diffusion are:

$$\varepsilon = \ell_0; P(t,\ell_0) \equiv P_{in}(t); P_A(t,\varepsilon_{\max}) \equiv 0; \tag{15}$$

The numerical algorithm of the solutions to this model problem has peculiarities in the sequence of the nodal points in that the spatial coordinate is strongly compressed from the right. In this connection, the application of an uneven network in the space is obviously useful, which is naturally realized according to Eq. (11).

IV. CONCLUSIONS

Effective was the application of the concept of fractals for the mathematical modeling of the structure of porous materials. This application facilitated the establishment of differential equations for the kinetics of adsorption of gases on the inner surface of the adsorbent.

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